

Role of input atomic data in spectroscopic analyses of the Sun and metal-poor stars

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Abstract.

Analysis of high-resolution stellar spectra relies heavily upon atomic data. These include energy levels, wavelengths, cross-sections for various types of interactions between particles and photons, such as photoionization and collision induced transitions. Quantum-mechanical calculations provide largest part of these data. In this paper I describe atomic data necessary to compute model atmospheres and line formation for the late-type stars both in the assumption of local thermodynamic equilibrium (LTE) and in a more general case of non-LTE. I will focus on transition metals with $21 < Z < 29$ and discuss whether (and where) more complete and/or accurate atomic data are necessary.

1. Introduction

Chemical composition of late-type (FGK) stars provides major observational constraints to the chemical evolution of the Galaxy. These stars span a huge range of metallicities and ages and, due to relatively cool surfaces, their spectra are rich in lines of different atomic and molecular species that allows to determine abundances of many chemical elements. For certain elements, lines due to forbidden and dipole-allowed transitions, as well as molecular lines, can be analysed simultaneously, e.g. [CI], CH, and C I.

At present, determination of element abundances usually proceeds in two steps. First, one constructs a model of a stellar atmosphere using basic conservation laws and certain simplifying assumptions, which are valid for a restricted range of stellar parameters. The model gives variation of basic atmospheric quantities, local kinetic gas temperature T_e and number density of free electrons N_e , as a function of depth. Next, the model is used to solve radiative transfer equation for individual spectral features to compare them with observations. In both steps, it is necessary to describe correctly absorptive properties of the atmospheric plasma, which depend on the distribution of atoms and ions among excitation states and ionization stages N_i , and on the cross-sections for interaction of gas particles with radiation field. In a simple case of *local thermodynamic equilibrium* (LTE), the former is computed from the Saha-Boltzmann equations for local values of T_e and N_e at each point of the model atmosphere. However, in reality atomic level populations N_i are, in return, affected by the radiation field, which is generally highly non-local due to scattering processes. Thus, N_i also depend on physical conditions at other depth points and must be determined from the solution of full equations of statistical equilibrium for each ion and each of its energy levels, an approach known as non-LTE. These equations must include the rates of all processes,

which represent interaction between particles and photons, such as radiatively-induced excitation and ionization of atoms. The need for accurate cross-sections of these processes renders atomic data as one of the key ingredients in stellar atmosphere studies.

Below, I will briefly describe atomic data necessary to compute model atmospheres and line formation both in LTE and non-LTE cases. I will focus on the late-type stars with $4000 < T_{\text{eff}} < 6500$ and $3 < \log g < 5$, and on transition metals with $21 < Z < 29$. Abundances of these elements in old stars provide key information for understanding explosive nucleosynthesis in supernovae. Brief reviews of atomic data used in precision stellar spectroscopy are also given in Johansson (2008) and Mashonkina (2009).

2. Opacity in model atmospheres and spectrum synthesis

Construction of theoretical model atmospheres requires a detailed knowledge of the monochromatic absorption coefficients over a huge frequency interval. For the range of stellar parameters corresponding to late-type stars, the following opacity sources are relevant. The continuous extinction is represented by the free-free transitions in H I, He⁺, H⁺, and H₂⁺, Rayleigh scattering for H, He, and H₂, and Thomson scattering on electrons. Also included are bound-free transitions in H⁺, H I, He I, H₂⁺ and H₂⁺. Very important absorbers in the UV and visual spectral range are C I, Mg I, Si I, Al I, Fe I. For these species it is crucial to have accurate photoionization cross-sections. Grupp (2004) showed that quantum-mechanical cross-sections for Fe I (Bautista 1997, Iron project) lead to a much better agreement between theoretical and observed solar fluxes in the UV and IR spectral regions. The influence of Fe I bound-free opacity on the solar UV continuum fluxes was also demonstrated in Bell et al. (2001) using MARCS and ATLAS9 models, although they argued that the quantum-mechanical cross-sections should be increased by a factor of two to match the fluxes in the spectral range 3000...4000 Å. These same arguments may not apply to other types of atmospheric models.

Line opacity is dominated by bound-bound transitions in neutral and singly-ionized atoms of Fe-peak elements, although opacity due to other atoms (e.g. H I) and molecules (e.g. H₂, CH, OH, MgH, TiO) has to be included as well. Modern model atmosphere codes (e.g. MAFAGS: Grupp et al. 2009) use tens of millions of lines to construct opacity distribution functions or sample them at certain frequencies to save computational efforts. Recent calculations of Kurucz¹ increased the number of predicted radiative bound-bound transitions for several neutral atoms, such as Fe I, Ti I, Cr I to few millions; most of these transitions originate from the levels with very high excitation energies. Grupp et al. (2009) showed that including all predicted transitions has a small effect on the mean temperature structure of the solar atmosphere: up to 25 K in the line formation regions. Another interesting result was a reduced discrepancy between observed and synthetic solar fluxes in the UV.

3. Line formation

Calculation of synthetic profiles for comparison with observations is not trivial even under LTE and requires atomic data for individual lines: wavelengths, energies of

¹<http://kurucz.harvard.edu/>

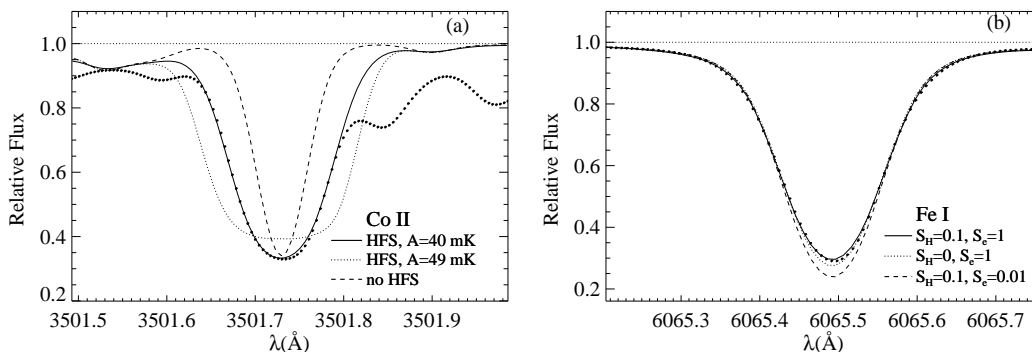


Figure 1. (a) The line of Co II in the solar KPNO flux spectrum (filled circles). The profile computed with $A = 49$ mK for the lower level a^5P_3 gives an excellent fit of the observed profile (black trace). The profiles computed neglecting HFS (dashed trace) or with the less accurate laboratory value $A = 40$ mK (dotted trace) are also shown. (b) The solar line of Fe I computed with various scaling factors to inelastic H I and e^- collisions, S_H respectively S_e . The observed profile is shown with filled circles.

lower levels of transitions, oscillator strengths, pressure broadening parameters, hyperfine splitting and isotopic shifts. For most of these parameters, data from laboratory measurements are usually available, however the accuracies are not always as good as desirable.

In calculations of abundances by the most reliable and rigorous method of spectrum synthesis, one derives the product of abundance and oscillator strength of a transition, $gf\epsilon$. Thus, in absolute abundance analyses of stars the accuracy of former is never better than the latter. In general, it is more difficult to measure accurate oscillator strengths for weak transitions (Nilsson et al. 2003); this is manifested in the fact that a typical error in experimental f -values of weak lines is of the order of 20% or more. Often one has to rely on oscillator strengths from different sources, affected by various sources of uncertainties.

In analyses of stars other than the Sun, there is a way to avoid gf -values completely. In the relative abundance analyses, oscillator strengths do not enter calculations at all, because any abundance estimate derived from a single line in a spectrum of a metal-poor star is referred to that from same line in a spectrum of a reference star, e.g. the Sun. However, this works well on condition that for both objects a line appears on the same part of the curve-of-growth and, thus, is equally sensitive to various atmospheric quantities (abundance, pressure and turbulent broadening). This is true only for a very limited range of stellar parameters.

Some lines are affected by hyperfine splitting (HFS) and/or isotopic shift, and these types of line “broadening” are comparable or even larger than the thermal broadening of lines at local kinetic temperatures in the atmospheres of solar-type stars. HFS is particularly pronounced for odd- Z elements Mn and Co with large atomic masses and large nuclear spins, $5/2$ respectively $7/2$. The effect of HFS is to de-saturate spectral lines leading to a compound profile, where the strength of each component is linearly propor-

tional to the element abundance. To compute accurate separation of HFS components, magnetic dipole constants A must be known with an accuracy of at least 10%. Fig. 1 shows that the Co II line at 3501 Å computed with an approximate estimate $A = 49$ mK for its lower level a^5P_3 (Pickering et al. 1998) cannot fit the observed profile at all. In contrast, a more accurate laboratory value $A = 40$ mK from Bergemann et al. (2010) provides an excellent fit to the observed profile. A profile computed without HFS is also shown.

Finally, accurate wavelengths of transitions are important in studies of line asymmetries (Dravins et al. 1981; Nordlund & Dravins 1990), e.g. in diagnostic analyses by means of 3D hydrodynamical model atmospheres and for identification of blending features.

3.1. NLTE radiative transfer

Computing NLTE line formation is very time-consuming and complex compared to LTE, because much more atomic data are necessary in addition to the standard set of parameters for individual lines as described above.

Atomic models for statistical equilibrium calculations must be fairly complete. Various processes representing interaction between atoms, electrons, and radiation are to be included. These are photon absorption in line transitions, photoionization, excitation and ionization by collisions with free electrons and neutral hydrogen atoms. All processes include their reverse reactions; for scattering in discrete radiative transitions, one usually assumes complete frequency redistribution. The current status of NLTE modelling for neutral atoms of transition metals is described below. These elements have a partly filled $3d$ subshell that gives rise to fairly complicated but interesting atomic properties.

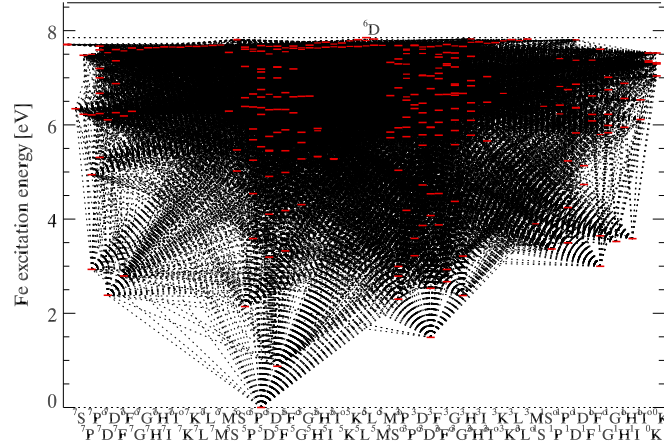


Figure 2. Grotrian diagram of the Fe I atom constructed using the new predicted levels and transitions from the Kurucz's database. The ground state of the Fe II, a^6D , is indicated.

The number of levels and discrete radiative transitions in neutral atoms of the Fe-group is enormous. Recent calculations of Kurucz predict tens of thousands of levels and few millions of transitions. Such atomic models are not tractable even with 1D NLTE codes; thus, recently, we developed efficient algorithms to combine atomic levels and transitions into super-levels and super-lines in a way that a reduced model atom inherits the basic properties of the complete model and has similar performance under restriction of different stellar parameters. For example, application of these algorithms to Fe I reduced the number of levels from 37 500 to 292, and the number of radiative bound-bound transitions from $\sim 6\,029\,000$ to 13600 (Fig. 2). Furthermore, for 3D NLTE calculations, we have constructed a model with 172 levels and 1120 transitions, which is now being tested in 1D and 3D NLTE line formation codes. The requirements to the accuracy of transition probabilities, or f -values, are not very strict. Strong lines, which are subject to non-equilibrium excitation effects, have laboratory f -values with 5 – 10% accuracy. For transitions between a bulk of intermediate- and highly-excited levels, the accuracy of 20–30% is sufficient, because the energy separation of the levels is in most cases small enough for collisions to dominate over radiative rates.

The situation is more uncertain for bound-free radiative processes. Hydrogenic approximation is usually adopted for photoionization; however comparison with quantum-mechanical data for Fe I (Bautista 1997) and Cr I (Nahar 2009) shows that the former is not correct even within an order of magnitude. The quantum-mechanical cross-sections for the levels of both atoms are larger in the background and are characterised by prominent resonances that leads to significantly enhanced ionization rates in statistical equilibrium calculations and, thus, to different abundances. In some cases, accurate position of resonances is important, because UV radiation field varies strongly with frequency in the atmospheres of late-type stars and ionization rates may change depending on whether a resonance appears at energies with high or low fluxes. Available laboratory data very sparse; e.g. for a few Ti I intermediate-excitation levels the cross-sections were measured by Yang et al. (2009) by the method of resonance ionization mass spectrometry. Experimental values are very useful to check the accuracy of theoretical values for individual transitions, however they cannot cover the complete atomic system that is essential in NLTE calculations of atomic level populations for stellar atmosphere studies. Thus, quantum-mechanical data are indispensable.

Cross-sections for H I and e^- collisions are basically unknown. Thus, we have to rely on commonly-used approximations or to neglect these processes completely. Cross-sections for continuum and allowed discrete transitions due to inelastic collisions with H I are computed with the formulas of Drawin (1968, 1969a,b). This recipe was originally developed for collisions between equal atoms, H and Ar, and later it was extended to Li-H collisions by Steenbock & Holweger (1984). The rates of allowed and forbidden transitions due to collisions with electrons are calculated from the formulae of van Regemorter (1962) and Allen (1973), respectively. Bound-free transitions caused by electron collisions are treated according to Seaton (1962). Similar to photoionization, the accuracy of the data obtained with these formulae is very low. Comparison of R-matrix calculations for e^- collisions for Ca II (Meléndez et al. 2007) with the formula of van Regemorter (1962) reveals order of magnitude differences. What concerns inelastic H I collision, compared to the Drawin's formulae, ab initio quantum-mechanical calculations predict significantly lower collision rates for certain transitions of simple alkali atoms (Belyaev & Barklem 2003; Barklem et al. 2010), and they show that, in addition to excitation, other effects like ion-pair formation become important. Excitation and ionization balance in the atoms of the Fe-group depend on e^- collision

efficiency for solar-type stars, i.e. metallicities $[\text{Fe}/\text{H}] \geq -0.5$. In the atmospheres of metal-poor stars, where NLTE effects on abundances are large, collisional excitation is fully controlled by neutral hydrogen.

The deficiencies in NLTE models often reveal themselves, when synthetic spectra are compared with observations, e.g. by producing large abundance discrepancies between different spectral lines of the same atom. Thus, it is common to introduce scaling factors, which are adjusted to obtain agreement between various spectral lines. Fig. 1b shows the profiles of the solar Fe I line computed with different scaling factors to Drawin's H I collision rates, $S_{\text{H}} = 0, 0.1$. Inelastic e^- collision rates computed using the formulae of van Regemorter (1962) and Seaton (1962) are also scaled by $S_{\text{e}} = 0.01, 1$. The figure shows that a proper choice of S_{H} and S_{e} may also remove discrepancy between observed and synthetic line profiles.

4. Discussion and outlook

The calculations of NLTE stellar spectra for the late-type stars are usually decoupled from calculations of model atmospheres. As a rule, the latter are computed assuming LTE, and line formation calculations are performed keeping the input model fixed. Such a “simplified” NLTE approach is not fully justified, because various elements affect the structure of the atmosphere by contributing free electrons and/or opacity, such as Mg, Al, Si, Fe, Ti (see Sec. 2). Deviations from LTE in the excitation and ionization equilibria of these elements will lead to changes in the energy balance. Thus, NLTE rate equations for all these elements must be solved simultaneously in model atmosphere calculations, a numerically challenging task. Another problem is that atomic data for some of these elements are of very low quality or lack completely. This refers to photoionization, H I and e^- impact excitation and ionization cross-sections.

The first problem has been successfully overcome with enormous progress in numerical techniques and computing facilities in the past 10 years. At present it is possible to compute NLTE line-blanketed model atmospheres (Anderson 1989; Short & Hauschildt 2005a; Haberreiter et al. 2008). These and other studies proved the importance of NLTE effects on the atmospheric structure and spectral energy distributions for the Sun (Short & Hauschildt 2005a) and non-negligible differences for metal-poor stars (Short & Hauschildt 2005b). There is no doubt that soon self-consistent NLTE models will replace LTE-based ones; accurate atomic data will stimulate and, thus, accelerate this transition.

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